THEORETICAL NEUTRON-CAPTURE CROSS SECTIONS FOR R-PROCESS NUCLEOSYNTHESIS IN THE ^{48}CA REGION

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Abstract:

We calculate neutron capture cross sections for r-process nucleosynthesis in the ^{48}Ca region, namely for the isotopes $^{40-44}$S, $^{46-50}$Ar, $^{56-66}$Ti, $^{62-68}$Cr, and $^{72-76}$Fe. While previously only cross sections resulting from the compound nucleus reaction mechanism (Hauser-Feshbach) have been considered, we recalculate not only that contribution to the cross section but also include direct capture on even-even nuclei. The level schemes, which are of utmost importance in the direct capture calculations, are taken from quasi-particle states obtained with a folded-Yukawa potential and Lipkin-Nogami pairing. Most recent deformation values derived from experimental data on β-decay half lives are used where available. Due to the consideration of direct capture, the capture rates are enhanced and the "turning points" in the r-process path are shifted to slightly higher mass numbers. We also discuss the sensitivity of the direct capture cross sections on the assumed deformation.

1 Introduction

A number of investigations (see e.g. [1,2]) of the nuclear properties of neutron rich nuclei close to and at the magic neutron number $N = 28$ has been motivated by the fact that these isotopes may play a crucial role in explaining the Ca-Ti-Cr-Fe isotopic anomalies found in meteoritic inclusions. Experimental information is scarce due to the short half-life of the involved nuclei. However, β-decay properties of several isotopes in that region have been measured [1,3,4] recently. Theoretical predictions can be improved by utilizing such experimental data.

For the isotopes ^{43}P, ^{42}S, ^{44}S, ^{45}S, ^{44}Cl, ^{45}Cl, ^{46}Cl, and ^{47}Ar, nuclear deformations have been derived from the measured β-decay half-lives in a recent QRPA parameter study [3,4]. Taking these

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deformations we calculated the QP-levels below and close to the neutron separation energy, which are needed as input for the determination of the capture cross sections. However, we also extended our calculations to more neutron rich isotopes of S and Ar, and to Cr-, Ti- and Fe-isotopes by taking the deformations from a theoretical mass formula [5]. With this level information we updated the theoretical cross sections of the even-even isotopes of $^{40-44}$S, $^{46-50}$Ar, $^{56-66}$Ti, $^{62-68}$Cr, and $^{72-76}$Fe. The importance of – and the accuracy in the reproduction of experimental data by – direct capture for the case of ^{48}Ca was already shown elsewhere [6].

2   Method

Mainly two reaction mechanisms have to be considered for astrophysically relevant neutron energies: the Compound Nucleus Mechanism (CN, Hauser-Feshbach, statistical model) and Direct Capture (DC) to bound states. For the majority of neutron-rich intermediate and heavy mass nuclei CN will dominate. However, the statistical model is only applicable as long as the level density is sufficiently high (i.e. ≥ 10 MeV^{-1}). Therefore, DC may dominate for capture on nuclei with low level densities at the neutron separation energy. This can be the case for light nuclei, nuclei close to magic neutron numbers, and nuclei close to the neutron drip line (similar for proton capture on the proton rich side).

In previous r-process network calculations [1] only CN was considered in the theoretical neutron capture cross sections for the relevant nuclear region. Moreover, the level densities were computed from a back-shifted Fermi-gas formula [7]. For our purposes we calculated quasi-particle levels in a folded-Yukawa potential and with Lipkin-Nogami pairing [5]. The levels derived in such a way were used as input for the statistical model code SMOKER [8] and for the direct capture code TEDCA [9].

After the calculation of the nuclear energy levels and the CN cross sections, the DC contributions for capture on even-even nuclei (to first order one can assume that the level density in nuclei with one or two unpaired nucleons will be higher than for even-even nuclei, and that therefore DC will be most important for capture on even-even targets) were determined as follows. The theoretical cross section σ^{th} is given by a sum over each final state i [10]

$$\sigma^{\mathrm{th}} = \sum_i C_i^2 S_i \sigma_i^{\mathrm{DC}} \quad . \tag{1}$$

In our case the isospin Clebsch-Gordan coefficients C_i are equal to unity. The spectroscopic factors S_i describe the overlap between the antisymmetrized wave functions of target+n and the final state. In the case of one-nucleon capture on even-even deformed nuclei, the spectroscopic factor for capture into a state i, which has an occupation probability v_i^2 in the target, can be reduced to [11]

$$S_i = 1 - v_i^2 \quad . \tag{2}$$

The corresponding probabilities v_i^2 are found by solving the Lipkin-Nogami pairing equations [5].

The factors σ_i^{DC} in Eq. 1 are essentially determined by the overlap of the scattering wave function in the entrance channel, the bound-state wave function and the multipole-transition operator. The

potentials needed for the calculation of the before-mentioned wave functions are obtained by applying the folding procedure. In this approach, the nuclear density of the target ρ_T is folded with an energy and density dependent effective nucleon-nucleon interaction w_{eff} [12]

$$V(E, R) = \lambda V_F(E, R) = \lambda \int \rho_T(\vec{r}) w_{\text{eff}}(E, \rho_T, |\vec{R} - \vec{r}|) \, d\vec{r} \quad , \tag{3}$$

with $\vec{R}$ being the separation of the centers of mass of the two colliding nuclei. The interaction w_{eff} is only weakly energy dependent in the energy range of interest [13]. The density distributions ρ_T were calculated from the folded-Yukawa wave functions.

The only remaining parameter λ was determined by employing a parametrization of the volume integral I

$$I(E) = \frac{4\pi}{A} \int V_F(R, E) R^2 \, dR \quad , \tag{4}$$

expressed in units of $\text{MeV} \, \text{fm}^3$, and with the mass number A of the target nucleus. Recently, the averaged volume integral I_0 was fitted to a function of mass number A, charge Z and neutron number N for a set of specially selected nuclei: [14]

$$I_0 = 255.13 + 984.85 A^{-1/3} + 9.52 \times 10^6 \frac{N - Z}{A^3} \quad . \tag{5}$$

Thus, the strength factor λ can easily be computed for each nucleus by using

$$\lambda = \frac{I_0}{I} \quad . \tag{6}$$

For the bound states, the parameters λ are fixed by the requirement of a correct reproduction of the separation energies.

3 Results and Discussion

The calculated CN and DC cross sections as well as the deformation parameters used for the calculation of the single-particle levels are shown in Table 1. The quoted neutron separation energies in the final nucleus are taken from an experimental compilation [15] where available, otherwise they were calculated from the theoretical mass formula [5]. Furthermore, β-decay half-lives are compared to theoretical lifetimes against neutron capture, computed from our results with a neutron number density of 3×10^{19} cm^{-3} (S, Ar) and 6×10^{20} cm^{-3} (Ti, Cr, Fe). Shown are experimental β-decay properties [1,3,4] and also theoretical values obtained by using the QRPA code [16] with folded-Yukawa wave functions and Lipkin-Nogami pairing for nuclei for which no experimental β-decay properties were known.

From Table 1 one can see nicely the importance of direct capture when approaching the magic neutron number $N = 28$ (S, Ar), but also the increasing contribution of DC to the cross section when approaching the drip line. The latter point can clearly be seen for the Ti isotopes and coincides well with the drop in level density at the neutron separation energy. The calculated Cr isotopes are still farther away from the drip line, therefore the capture cross section is dominated by CN.

Table 1: Calculated 30 keV (c.m.) Maxwellian averaged neutron capture cross sections $< \sigma >_{30\,\text{keV}}$ for CN and DC. The column labeled '%' gives the portion of direct capture in the total cross section. Also shown are the deformations ϵ_2 and neutron separation energies S_n of the final nucleus target+n. The neutron capture half-lives $T_{1/2}(n)$ were computed with the values from column 'DC+CN' and a neutron number density of 3×10^{19} (S, Ar) and 6×10^{20} cm^{-3} (Ti, Cr, Fe), respectively.

Target	ϵ_2	S_n [MeV]	DC [mb]	CN [mb]	DC+CN [mb]	%	$T_{1/2}(n)$ [s]	$T_{1/2}(\beta)$ [s]
^{40}S	+0.24	3.8238‡	0.4246	0.0851	0.5097	83	0.218	8.60
^{42}S	+0.30*	3.3114‡	0.9466	0.0202	0.9668	98	0.115	0.56±0.06†
^{44}S	−0.20*	1.3344	0.0000	0.0044	0.0044	0	25.25	0.12±0.01†
^{44}S^a	+0.30	1.3344	0.014	0.0044	0.0184	76	6.040	0.12±0.01†
^{46}Ar	−0.18*	4.2590‡	0.5295	0.1203	0.6498	81	0.171	7.80
^{48}Ar	−0.22	1.7074	0.0427	0.0144	0.0571	75	1.946	0.11
^{50}Ar	−0.28	1.0804	0.0016	0.0030	0.0046	35	24.15	0.05
^{56}Ti	+0.13	2.1936‡	0.0147	0.1305	0.1452	10	0.038	0.421
^{58}Ti	−0.10	2.4244	0.0185	0.0797	0.0982	19	0.057	0.152
^{60}Ti	−0.02	2.1194	0.0165	0.0403	0.0568	29	0.098	0.054
^{62}Ti	−0.04	0.5878	0.0068	0.0030	0.0098	69	0.569	0.018
^{64}Ti	+0.06	0.4094	0.0013	0.0002	0.0015	87	3.561	0.039
^{66}Ti	+0.14	0.3914	0.0009	0.0002	0.0011	82	4.960	0.013
^{62}Cr	+0.30	2.9134	0.0119	0.3846	0.3965	<1	0.014	0.349
^{64}Cr	+0.05	1.8614	0.0170	0.0353	0.0523	33	0.106	0.154
^{66}Cr	+0.10	2.2374	0.0126	0.0673	0.0799	16	0.071	0.071
^{68}Cr	+0.16	1.8274	0.0129	0.0268	0.0397	32	0.140	0.026
^{72}Fe	+0.14	2.2474	0.0101	0.0572	0.0673	15	0.083	0.089
^{74}Fe	+0.07	2.0564	0.0104	0.0360	0.0464	22	0.120	0.052
^{76}Fe	+0.06	0.0584	0.0050	3×10^{-6}	0.0050	>99	1.12	0.045

^{a} $\epsilon_2(^{45}\text{S})=\epsilon_2(^{44}\text{S})= +0.3^*$ (see text)

* deformation inferred from experimental β-decay half-life [3,4]

† experimental β-decay half-life [1,3,4]

‡ S_n from experimental values [15]

Table 2: Quasi-particle levels for ^{44}S and ^{45}S.

^{44}S ($\epsilon_2 = +0.3$)		^{45}S ($\epsilon_2 = -0.2$)	
E_x [MeV]	[Nn$_z\Lambda$]Ω	E_x [MeV]	[Nn$_z\Lambda$]Ω
-27.1979	[0 0 0] 1/2	-26.0041	[0 0 0] 1/2
-20.3364	[1 1 0] 1/2	-18.2826	[1 0 1] 3/2
-17.8157	[1 0 1] 3/2	-17.6452	[1 1 0] 1/2
-15.8641	[1 0 1] 1/2	-15.5487	[1 0 1] 1/2
-12.4255	[2 2 0] 1/2	-10.3816	[2 0 2] 5/2
-10.3579	[2 1 1] 3/2	-9.2965	[2 1 1] 3/2
-7.8438	[2 0 2] 5/2	-8.9932	[2 2 0] 1/2
-7.5158	[2 0 0] 1/2	-5.8346	[2 0 0] 1/2
-4.1707	[2 1 1] 1/2	-5.7213	[2 0 2] 3/2
-3.9511	[3 3 0] 1/2	-3.0690	[2 1 1] 1/2
-3.2493	[2 0 2] 3/2	-1.7317	[3 0 3] 7/2
-2.3583	[3 2 1] 3/2	-0.6623	[3 1 2] 5/2
-0.5604	[3 1 2] 5/2	-0.3329	[3 2 1] 3/2
0.0000	[3 1 0] 1/2	-0.1400	[3 3 0] 1/2
0.0582	[3 0 3] 7/2	0.0000	[3 0 1] 3/2
0.9147	[3 2 1] 1/2	0.5831	[3 1 0] 1/2
		1.2550	[3 0 3] 5/2

An interesting effect can be seen for ^{44}S: DC is suppressed totally when assuming a deformation $\epsilon_2(^{45}$S$)= -0.2$, as suggested in order to reproduce the experimental β-decay half-life [3,4] of ^{45}S. Due to the different deformations of target ($\epsilon_2(^{44}$S$)= +0.3$) and final nucleus, the level order is changed and the previously unbound [303]7/2$^-$ level (E_x=0.0582 MeV) is shifted well below the Fermi energy in ^{45}S. This means that not only is a captured neutron added to one level of ^{44}S, but also that the nucleus is undergoing a reordering process. Such a process cannot be described by DC and therefore the respective cross section will vanish. As found in the QRPA parameter study [3,4], another deformation value consistent with the experiment would be $\epsilon_2(^{45}$S$)= +0.125$. However, even with this value a similar effect can still be seen. Only with a deformation very close to the deformation of the target nucleus, non-zero DC cross sections can be obtained. Nevertheless, one has to note that the calculated QP levels might have an uncertainty which is larger than the distance of the level in question from the Fermi energy. Therefore, it might still be reasonable to calculate a DC contribution by assuming the same deformation for target and final nucleus. The resulting cross sections for the two cases $\epsilon_2(^{45}$S$)= -0.2$ and $\epsilon_2(^{45}$S$)= +0.3$ are shown in Table 1. The level schemes for ^{44}S and ^{45}S are shown in Table 2. The astrophysical consequences are not changed for either deformation because the neutron capture lifetime is longer by orders of magnitude than the β-decay lifetime in both cases.

4   Summary

It has been shown that it is important to consider DC cross sections as well as CN cross sections for nuclei close to magic numbers and close to the drip lines. However, in order to reliably calculate

DC contributions one needs level schemes which can be calculated from microscopic models. In this context, improved experimental data is of utmost importance not only for a better knowledge of β-decay half-lives, but also to be able to infer deformation parameters. With our new neutron capture cross sections we obtain "turning points" in the r-process path for the mentioned neutron densities at ^{44}S, ^{48}Ar, ^{62}Ti (with a minor branching at ^{60}Ti), ^{68}Cr (^{66}Cr), and ^{74}Fe (^{72}Fe). (Note, however, that the theoretical β-decay half-lives shown are taken from QRPA calculations [16]. Other models might yield different values). Full reaction network calculations with varying neutron densities have to be performed for a more detailed determination of the resulting abundances and isotopic ratios.

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